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Structural domain walls in polar hexagonal manganites¹

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The domain structure in the multiferroic hexagonal manganites is currently intensely investigated, motivated by the observation of intriguing sixfold topological defects at their meeting points [Choi, T. et al., *Nature Mater.* 9, 253 (2010).] and nanoscale electrical conductivity at the domain walls [Wu, W. et al., *Phys. Rev. Lett.* 108, 077203 (2012).; Meier, D. et al., *Nature Mater.* 11, 284 (2012).], as well as reports of coupling between ferroelectricity, magnetism and structural antiphase domains [Geng, Y. et al., *Nano Lett.* 12, 6055 (2012).]. The detailed structure of the domain walls, as well as the origin of such couplings, however, was previously not fully understood. In the present study, we have used first-principles density functional theory to calculate the structure and properties of the low-energy structural domain walls in the hexagonal manganites [Kumagai, Y. and Spaldin, N. A., *Nature Commun.* 4, 1540 (2013).]. We find that the lowest energy domain walls are atomically sharp, with $\{210\}$ orientation, explaining the orientation of recently observed stripe domains and suggesting their topological protection [Chae, S. C. et al., *Phys. Rev. Lett.* 108, 167603 (2012).]. We also explain why ferroelectric domain walls are always simultaneously antiphase walls, propose a mechanism for ferroelectric switching through domain-wall motion, and suggest an atomistic structure for the cores of the sixfold topological defects.

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